



SCIEX OS 1.2

Release Notes



This document is provided to customers who have purchased SCIEX equipment to use in the operation of such SCIEX equipment. This document is copyright protected and any reproduction of this document or any part of this document is strictly prohibited, except as SCIEX may authorize in writing.

Software that may be described in this document is furnished under a license agreement. It is against the law to copy, modify, or distribute the software on any medium, except as specifically allowed in the license agreement. Furthermore, the license agreement may prohibit the software from being disassembled, reverse engineered, or decompiled for any purpose. Warranties are as stated therein.

Portions of this document may make reference to other manufacturers and/or their products, which may contain parts whose names are registered as trademarks and/or function as trademarks of their respective owners. Any such use is intended only to designate those manufacturers' products as supplied by SCIEX for incorporation into its equipment and does not imply any right and/or license to use or permit others to use such manufacturers' and/or their product names as trademarks.

SCIEX warranties are limited to those express warranties provided at the time of sale or license of its products and are SCIEX's sole and exclusive representations, warranties, and obligations. SCIEX makes no other warranty of any kind whatsoever, expressed or implied, including without limitation, warranties of merchantability or fitness for a particular purpose, whether arising from a statute or otherwise in law or from a course of dealing or usage of trade, all of which are expressly disclaimed, and assumes no responsibility or contingent liability, including indirect or consequential damages, for any use by the purchaser or for any adverse circumstances arising therefrom.

For research use only. Not for use in diagnostic procedures.

AB Sciex is doing business as SCIEX.

The trademarks mentioned herein are the property of AB Sciex Pte. Ltd. or their respective owners.

AB SCIEX™ is being used under license.

© 2017 AB Sciex



AB Sciex Pte. Ltd.
Blk 33, #04-06
Marsiling Ind Estate Road 3
Woodlands Central Indus. Estate.
SINGAPORE 739256

Contents

Chapter 1 Introduction.....	4
New Features.....	4
Technical Support.....	5
Contact Us.....	5
Required Software.....	5
Operating System Requirements.....	5
Installation Instructions.....	6
Install the Software.....	6
Upgrade from Previous Versions of SCIEX OS.....	6
Install Optional Vertical Applications.....	7
Mass Spectrometer Firmware Versions.....	8
Instrument Configuration Table.....	8
Downgrade to Previous Versions of the Software.....	8
Computer Requirements.....	8
Fixed Issues.....	8
New Features and Fixes from Version 1.0 to Version 1.1.....	9
Chapter 2 Notes on Use and Known Issues.....	11
Revision History.....	31

Thank you for choosing SCIEX to supply your system. We are pleased to give you SCIEX OS 1.2 that supports both the SCIEX X500R QTOF and the SCIEX X500B QTOF systems, which provide liquid chromatography-time-of-flight mass spectrometry functions.

This document contains instructions for installing the software, describes features in the software, and provides troubleshooting guidelines. Keep these release notes for your reference as you become familiar with the software.

Note: The numbers in parentheses are reference numbers for each issue or feature in our internal tracking system.

New Features

- Significant improvement were made in performance speeds for peak review and data processing for large data sets in the Analytics workspace.
 - The performance time to open and process large data files in the Results Tables acquired in version 1.2 has improved.

Note: The performance time to open and process data files acquired in version 1.1 or 1.0 remains the same.

- The processing method steps in AutoPeak have been optimized, decreasing the time to create processing methods. (MQ-2271)
- Users can now create and export a MarkerView™ software compatible peak list file. The file contains peak information from the Results Table (mass, intensity, and so forth). After the list is created, it can be imported to MarkerView™ software for PCA and other statistical analysis. (MQ-2087)
- Query functionality has been added to Reporter templates. For example, the Analyte 20 percent report template and query have been added to the Analytics workspace. The report shows a section that includes the File Information for each analyte and an XIC table for each Blank, Standard, QC, and 20% of all the unknown samples. The unknown samples are selected by the user-defined criteria in the report query. (MQ-2179)
- Acquisition continues when processing data sets that require substantial computer processing resources. Processing might be paused to accommodate acquisition and will continue when processing resources become available.
- Users can now delete multiple individual batches or a range of batches from the queue. (ACQ-2576, ACQ-2483)

- Sample Name and Sample ID fields in the Batch workspace now accept up to 252 characters and previously invalid special characters "\ / : * ? " < > | = " as valid characters. (ACQ-2577)

Analytics Workspace

Processing algorithms improvement to determine the "Found at" m/z ratio value for qualitative analysis in targeted and non-targeted workflows. To maximize the functionality of the Analytics workflows, we recommend reprocessing data acquired in earlier versions of the software.

Technical Support

SCIEX and its representatives maintain a staff of fully-trained service and technical specialists located throughout the world. They can answer questions about the system or any technical issues that might arise. For more information, visit the Web site at sciex.com.

Contact Us

SCIEX Support

- sciex.com/contact-us
- sciex.com/request-support

Customer Training

- In North America: NA.CustomerTraining@sciex.com
- In Europe: Europe.CustomerTraining@sciex.com
- Outside the EU and North America, visit sciex.com/education for contact information.

Online Learning Center

- SCIEXUniversity

Required Software

Microsoft Word 2013 is required for the report functionality in the Analytics workspace.

Operating System Requirements

- Microsoft Windows 7 64-Bit, SP1
- English (Language and Keyboard settings)

Installation Instructions

Install the Software

If the software must be installed from a DVD, then always install the software from the official DVD and confirm after the installation that the correct version is installed.

1. Log on to the computer as a Microsoft Windows user with Administrator privileges.
2. Do one of the following:
 - If the software is being installed from a DVD, then load the DVD in the DVD drive and continue with step 5.
 - If the software is being installed from a downloaded file, then continue with step 3.
3. Download the required .zip file from the SCIEX Web site.

Tip! To prevent potential installation issues, save the file to the D drive.

4. After the download is complete, right-click the downloaded file and then click **Extract All**.
5. Browse to the extracted files or the DVD and then double-click **Setup.exe**.
6. Follow the on-screen instructions.

The initial setup might take several minutes as the SQL server must be installed.
7. After the software is installed, restart the computer.
8. Start the software.
9. Type the license key in the appropriate field.

The license key comes with the system. If a license key is not available, then contact sciex.com/request-support
10. Complete the software activation screen.

Licenses are required for the Bio Tool Kit and ChemSpider features. Make sure to obtain licenses before attempting to use the features in the Explorer workspace.

Upgrade from Previous Versions of SCIEX OS

Use this procedure to upgrade from the following versions: SCIEX OS 1.0 plus SCIEX OS 1.0 HotFix 1 or SCIEX OS 1.1.

Note: Some of the steps might take some time to complete.

1. Log on to the computer as a Microsoft Windows user with Administrator privileges.

2. For acquisition computers do the following:
 - a. Open the currently installed SCIEX OS.
 - b. Open the MS Tune workspace.
 - c. Click **Positive MS Tuning**.
 - d. Click **Save Tuning Settings** in the left panel and then click **Save Settings**.
3. Back up the SCIEX OS data folder.

Data files created using SCIEX OS 1.2 cannot be used with SCIEX OS 1.1 or earlier versions.
4. Do one of the following:
 - If the software is being installed from a DVD, then load the DVD in the DVD drive and continue with step [7](#).
 - If the software is being installed from a downloaded file, then continue with step [5](#).
5. Download the required .zip file from the SCIEX Web site.

Tip! To prevent potential installation issues, save the file to the D drive.

6. After the download is complete, right-click the downloaded file and then click **Extract All**.
7. Browse to the extracted files or the DVD and then double-click **Setup.exe**.
8. Follow the on-screen instructions.

The initial setup might take several minutes as the SQL server must be installed.
9. After the software is installed, restart the computer.
10. For acquisition computers, run the MS FW Updater Utility. Refer to the MS FW Updater Utility READ ME file that comes with the software installation package.

Install Optional Vertical Applications

The following optional applications must be installed after the SCIEX OS is installed. If the application is not installed, then the software tile will not be shown on the home page.

BioPharmaView™ software version 2.1, MarkerView™ software version 1.3.1, and LibraryView™ software version 1.2 must be installed after SCIEX OS is upgraded to version 1.2.

Note: If newer versions of the applications are available, then contact sciex.com/request-support to verify software compatibility.

1. Install SCIEX OS.
2. Make sure that SCIEX OS is closed, and then install the BioPharmaView™, MarkerView™, or LibraryView™ software.

Introduction

3. Refer to the respective release notes for more information about installing the applications.

Mass Spectrometer Firmware Versions

Device	Firmware
Mass spectrometer	ATLAS_QTOF_ICX_v0_r03

Instrument Configuration Table

Device	Instrument Configuration Table
Mass spectrometer	X500R CONFIG_X500R_v0_r03 X500B CONFIG_X500B_v0_r02

Downgrade to Previous Versions of the Software

Contact sciex.com/request-support for help on downgrading from the current version of the software.

Computer Requirements

Dell OptiPlex XE2 computer, with:

- An Intel Core I5-4570S processor (Quad core, 2.90 GHz, 6 MB with HD Graphics 4600)
- 32 GB DDR3 1600 Mhz SDRAM
- 2*2 TB HDD (RAID1)
- DVD+-RW
- Computer specification required for acquisition computers: Two single-port Broadcom Ethernet cards

Fixed Issues

The following table contains issues fixed in version 1.2.

- Applying file permissions for a specific user causes the SCIEX OS to fail to start. (ACQ-2247)
- Shimadzu LC: The software only supports two pumps. (BLT-420)
- Advanced parameters are not fully saved in the MRM HR MS method. (MSCS-1034)
- The software stops responding if the user tries to expand a hidden column. (ACQ-2231)
- For MS methods that contain SWATH[®] acquisition and MRM HR experiments, the sort by precursor option in the MRM HR experiment is not enabled. (ACQ-2218)

- Values are copied twice when content is pasted in the Ion Reference Table. (ACQ-2241)
- The mass spectrometer goes to Fault state when running an acquisition while data is being processed. (DS-1015)
- The Ion Reference Table reverts to the first option in the Reference Table list, which prevents the batch from being submitted. (ACQ-2333)
- SWATH[®] acquisition methods can be modified during acquisition. (ACQ-2605)
- Processing does not complete during processing of complex data. (MQ-1883)
- Modifying the Center Mass (Da) in the Live Method window during a Q1 Tuning procedure and then saving those changed values during the Save Tuning Settings step might cause an error. (MSCS-1067)
- Generating the support package might take up to 15 minutes. (ACQ-2061)
- Running an acquisition method might cause an error message to be shown indicating that the memory available is insufficient to continue. (DS-907)
- In TOF MSMS scans, the CE value for the tri-fluoro acetic acid calibrant in the X500 ESI Negative Calibration Solution was set too high (–35V), causing the precursor ion to become unstable and fragment too easily. (ACQ-2806/2813, BLT-520/521)
- In the Analytics workspace, users cannot open a project folder that has project sub-folders that were created outside of the software. (MQ-1303/DS-1697)
- The detector was optimizing at 25 V above the optimal voltage setting. (ACQ-2826)

New Features and Fixes from Version 1.0 to Version 1.1

New Features

The Intact Protein Mode feature enables the analysis of intact proteins that are larger than 10 KDa.

LC auto calibration enables the calibration of the mass spectrometer by introducing the calibrant through the autosampler.

In the Analytics workspace, a new UV MS qualitative report is included. To function correctly, the suffix must be created in the Results Table along with the **compoundname** ms component.

Fixed Issues

- The software stops responding when the user cancels reprocessing of a Results Table generated using the non-targeting workflow. (MQ-1901)
- Pasting the Actual Concentration column results from one standard sample to another standard sample in the Results Table causes an error. (MQ-1513)

Introduction

- When users compare data between the Analytics workspace and the Explorer workspace, there might be differences between the results in, for example, the peak height and peak area. (BLT-427)
- If the user creates an IDA method, enables Dynamic CE for MS/MS using the default Dynamic Collision Energy Settings, and then saves the method, the Dynamic Collision Energy settings cannot be changed after the method is saved. (ONYX-1540)
- Calibration Parameter selection was done once using the first Calibration cycle instead of per cycle, using cycle-specific calibration. (BLT-427/BLT-407)
- Spectra could not be added to an existing library database. (BLT-402)
- IDA experiment ion intensities could be calculated incorrectly if insufficient candidate ions were selected. (BLT-435)
- Higher masses with significant intensities were observed outside of the designated Q1 selection window in SWATH[®] acquisition mode of the X500R system. (BLT-430)
- Data was inconsistent when users compared data that was acquired using and MRM HR methods that contained certain TOF mass ranges. (MSCS-1228)

Notes on Use

- For optimal performance, at least 20 GB of free disk space is required. Batches might not be acquired successfully if there is insufficient disk space. (DS-870)
- All default Ion Reference tables installed by SCIEX OS will be upgraded and any modifications made by the user will be lost if they were saved to the default filenames. We recommend saving the modified tables under different names. User-created custom tables will not be modified. When performing Auto-calibration in the Batch workspace using the CDS, the user must make sure to select the correct Ion Reference table for the corresponding CDS solution (that is, the names on the CDS bottles must match those of the Ion Reference tables). (BLT-441, ACQ-2527/2627, ONYX-1975)
- The following ESI calibration solutions are required for the SCIEX X500R QTOF and the SCIEX X500B QTOF systems before upgrading to SCIEX OS 1.2:

Solution	Part Number
FG* ESI POSITIVE CALIBRATION SOLUTION X500B	5049910
PTO* CALIBRATION SOLUTION SUITE FOR X500B SYSTEM	5033025
PTO* ESI POSITIVE CALIBRATION SOLUTION X500B 5 PACK	5032735

- Data files created in SCIEX OS 1.1 or earlier cannot be appended to data files acquired in SCIEX OS 1.2. Acquisition methods, batch files, data files, processing methods, and Results Tables or qsessions created or saved in SCIEX OS 1.2 are not supported in SCIEX OS 1.1 or earlier. (MQ-2321)
- In the Analytics workspace, users must open and then save existing methods to implement the updated isotopic abundance table. If an existing method is used without first opening the method, then the precursor mass calculation will not be updated and the results will be incorrect. To avoid any issues, do the following:
 1. Open the method. The precursor masses update automatically.
 2. Save the method using the same or new name. If the user clicks **Close**, then a message is shown, indicating that the method has been changed and that the user must save the method. (MQ-2183)
- To avoid performance issues or data corruption, do not perform any computer maintenance procedures, such as defragmentation or disk cleanup, during sample acquisition.

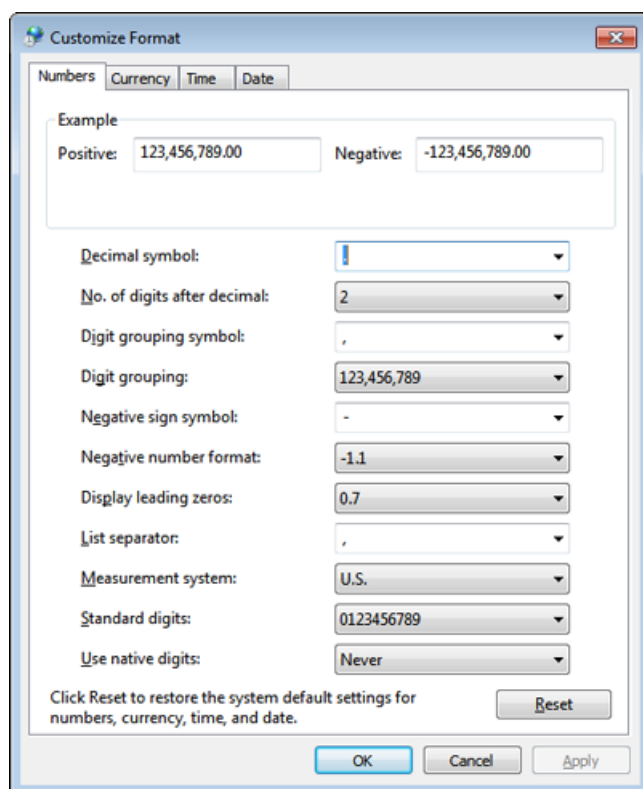
Notes on Use and Known Issues

- The latest version of the isotopic abundance table has been implemented. Any tables that use the atomic masses and isotopic abundances have been updated and, therefore, the average molecular mass calculation might change based on the revised calculation. (PV-1075)
- To avoid any installation issues, make sure that the path to the installation folder is not too long. If the data path is longer than 118 characters, then installation will not proceed.
- Set the anti-virus software to not scan during sample acquisition to avoid affecting system performance.
- When performing Windows updates, do not install any optional updates because they might impact functionality in the software.

Known Issues

The local settings shown in [Figure 2-1](#) are supported.

Figure 2-1 Local Settings



Label	Supported in SCIEX OS
Decimal symbol	Either '.' or ',' is supported.
No. of digits after decimal	Controlled by the number format in SCIEX OS.

Label	Supported in SCIEX OS
Digit grouping symbol	Not supported.
Digit grouping	Not supported.
Negative sign symbol	Controlled by SCIEX OS.
Negative number format	Not supported.
Display leading zeros	Not supported.
List separator	Not supported.
Measurement system	Not supported.
Standard digits	Not supported.
Use native digits	Not supported.

Table 2-1 General Issues

Issue	Description
In some rare instances, keyboard input is not accepted. (BLT-350)	<p>If this issue occurs, then start SCIEX OS again. Starting the software does not impact any ongoing data acquisition.</p> <hr/> <p>Tip! Users can copy and paste information in the fields, if required.</p> <hr/>
Microsoft Office cannot be installed after SCIEX OS is installed. (BLT-353)	<p>To avoid this issue, do the following:</p> <ol style="list-style-type: none"> 1. Install SCIEX OS. 2. Remove Microsoft Access. 3. Install Microsoft Office (32-bit). 4. Install Microsoft Access.

Notes on Use and Known Issues

Table 2-1 General Issues (continued)

Issue	Description
The correct status of a program that has been removed is only shown in the service package after the service package has been generated twice. (ACQ-2516)	To avoid any issues, generate the service package twice after a program is removed.
SCIEX OS 1.2 is not removed when a user tries to remove it using Setup.exe. (ONYX-2124)	If a user tries to remove SCIEX OS 1.2 using Setup.exe, the entry from Windows Programs and Features for SCIEX OS 1.2 is removed. However, the program remains and can still be opened. To remove SCIEX OS 1.2, run Setup.exe from SCIEX OS 1.2 folder and then follow the on-screen instructions to install the software. This process will add the entry for SCIEX OS back to the Windows Programs and Features list. Use the Programs and Features list to remove SCIEX OS 1.2.

Table 2-2 Devices

Issue	Description
Shimadzu LC: Incorrect device status is shown when the device is recovering. (ACQ-1410)	If a sub-device is turned off prior to sample submission, then the Shimadzu LC goes to Standby state even though the status should be Fault. If the user attempts to submit the batch to the queue again, then the first sample is submitted but fails immediately because the LC goes to Fault state and the sample becomes corrupted. If this issue occurs, then reset the computer and restart the software.
The system remains in Run state after recovery from MS communication loss during acquisition. (MSCS-432)	If the Ethernet cable is disconnected during acquisition, then the acquisition stops and the system goes to Fault state. After the Ethernet cable is connected again, if the user attempts to run another acquisition, then the acquisition completes and the real time display stops updating, but the system remains in Run state. If this issue occurs, then reactivate the device profile.
The calibrant delivery system (CDS) does not stop after the user starts it from Direct Control and then starts the queue with analytical samples. (ONYX-1428)	If the calibrant runs throughout the batch, then the sample might become contaminated with the calibrant. If this issue occurs, then stop the batch, stop the CDS, and start the batch again.
Agilent LC: The Fault state is not reflected correctly if the devices are in Fault state during device activation. (ACQ-2195)	To avoid this issue, clear the fault in the device, then deactivate and reactivate the Agilent devices.

Table 2-2 Devices (continued)

Issue	Description
Agilent LC: The comma is ignored as a decimal separator when the flow rate in the LC gradient grid is copied. (ACQ-2191)	This is an issue with the Agilent LC. To avoid this issue, manually type the flow rate, using a comma as the decimal separator.
Shimadzu and ExionLC LCs: The PDA default parameters are different depending on how the LC method is accessed. (ACQ-2176)	To avoid any issues, make sure that the correct parameters are used for the PDA device.
When the duration of a gradient table for an LC pump or column oven temperature table in an LC method is longer than the duration of the MS method, then the LC devices will stop running when the MS method duration expires. (ACQ-2167/2088)	To avoid this issue, make sure that the value in the Stop Time field for the LC method duration is the longest time that the LC method must run.
Agilent LC: During equilibration, if the user aborts the sample, then the Agilent LC might go to a Fault state. (ACQ-2142)	If this issue occurs, then click Standby to recover the device.
The software does not recognize the Queue option to proceed to the next sample if a sample vial is missing. (ACQ-1404)	To avoid this issue, the user must select the setting Ignore Missing Vessel in the Agilent system and then select the option If a sample is missing, then proceed to the next sample in the SCIEX OS Queue page in the Configuration workspace.
Shimadzu LC: The device traffic light does not update from Fault state when an error is recovered through Direct Control. (ACQ-1420)	If the user opens the Direct Control device and then clicks Clear Error when the LC is in Fault state, then the device recovers but the status in the software still indicates a fault. To clear this error, click Standby in the status panel.
The LC method does not run correctly if the devices that are turned on and connected do not match the devices in the activated device list. (ACQ-1716/2062)	To make sure that the system works correctly, either turn off the devices or turn on the devices to match the activated devices list.
Shimadzu LC: Inverted UV data is acquired during acquisition with two UV channels. (ACQ-2042)	This occurs when polarity is set to negative in the LC method UV detector section. To avoid any issues, use the positive setting for the polarity field.
Shimadzu LC: A performance issue is observed during running of a long batch using the Shimadzu PDA at sampling rates higher than 12.5 Hz. (ACQ-2037)	The expected duration of the batch might be longer than anticipated. To avoid any issues, use a sampling rate lower than 12.5 Hz.

Table 2-2 Devices (continued)

Issue	Description
Agilent LC: High throughput settings are not supported in the autosampler. (ACQ-529)	The high throughput settings are not currently supported.
Agilent LC: Agilent LC shows a Fault state even when the sub-devices have recovered from a fault and are in Ready state. (ACQ-2144)	If this issue occurs, then click Standby to return the LC to Ready state.
A system error is shown when there is a communication error between the devices and the mass spectrometer. (ACQ-2663)	If the batch is stopped, but the HPLC system continues to run, then the error message: CBM Disconnected is shown. This error might be caused by a communication error in the Shimadzu system. To avoid this issue, verify and set the IP address of the CBM to a unique ID and then inspect for any loose cable connections.
If the devices list contains a diverter valve and the user tries to acquire data using a method that does not contain a second step, then the acquisition stops. (MSCS-1284)	To avoid any issues, either make sure that the method has a switching step for the diverter or do not include a diverter valve in the devices list.
The system does not activate the Standby button on the right status panel when a subdevice, such as the CDS, goes to fault, preventing the user from clearing the error. (MSCS-1314)	If this issue occurs, then the user must go to CDS direct control and then click Start to change the CDS status from Fault to Running to clear the Fault status of the CDS subdevice.
The incorrect firmware version is shown in the Device Details dialog and Sample Information after the firmware and Configuration Table are upgraded. (ONYX-2056)	If this issue occurs, then <ol style="list-style-type: none"> 1. In the Devices panel, edit the mass spectrometer 2. Click Test Device. 3. Click Save.
SCIEX OS 1.2 is not removed when the user tries to remove it using Setup.exe. (ONYX-2124)	When a user tries to remove SCIEX OS 1.2 using Setup.exe, the entry from Windows Programs and Features for SCIEX OS 1.2 is removed. However, the program remains and can still be opened. To remove SCIEX OS 1.2, run Setup.exe from the SCIEX OS 1.2 folder and then follow the on-screen instructions to install the software. This process will add the entry for SCIEX OS back to the Windows Programs and Features list. Use the Programs and Features list to remove SCIEX OS 1.2.

Table 2-3 MS Methods

Issue	Description
The software does not save the required parameters when switching from an open method to another method after the ion source or probe is changed. (ACQ-2262)	If this issue occurs, then update the parameters, as required. Some parameters become unavailable if they are not required for the new ion source or probe.
The Method Editor grids resize beyond the available width. (ACQ-2243)	If this issue occurs, then use the scroll bars to access sections of the user interface that are not currently visible.
Only the grid parameters use the regional settings character for the decimal separator. (ACQ-2190)	Regional settings are followed in the MS Method and Batch grids, but not in the other fields in the MS Method Editor or the Equilibration dialog. To avoid any issues, use a period (".") as a decimal separator in all of the fields, excluding the MS Method and Batch grids.
No validation message is shown for the maximum number of windows per cycle in the Autofill SWATH Windows dialog. (ACQ-2296)	The maximum number of SWATH windows per cycle for an experiment is 200. If the options selected in the Autofill SWATH Windows dialog result in more than 200 windows per cycle being calculated, then the Windows per cycle field value is NA. The method cannot be generated. To avoid this issue, reduce the number of windows per cycle by increasing the Window width or by narrowing the difference between the Precursor start mass and the Precursor stop mass.
Ion source parameters are not updated to the mass spectrometer. (ACQ-2177)	During manual acquisition using a SWATH [®] and MRM HR method, the ion source gas and temperature parameters are available to be edited in the user interface. Users can edit the fields. However, the changes are not updated to the mass spectrometer nor are the changes logged in the sample information for that sample.
By default, the Apply Scan Schedule check box is selected in the MRM method that is generated when the Guided MRM HR feature is used. (ACQ-1681)	If this option is not required, then clear the check box before acquiring data using this method.

Notes on Use and Known Issues

Table 2-3 MS Methods (continued)

Issue	Description
The MS Method workspace does not update to show the correct information when running the calibrant. (ONYX-1556)	Although the user interface is not updated, the correct parameters are used and reflected in the file information.
If the user manually changes the decimal separator from period to comma in the Windows operating system and then also applies regional settings in SCIEX OS, then the following issues occur: <ul style="list-style-type: none">• The default values in the MS Method Editor numeric fields show periods as decimal separators instead of commas.• When the user edits the MS method, the numeric fields allow the user to type commas, but after the cursor is moved, the comma is not accepted. For example, the user types 0,25, but the value is entered as 25. (ONYX-2050)	To avoid any issues, use regional settings that use commas as the decimal separator, for example German.

Table 2-4 Acquisition

Issue	Description
When a Shimadzu LC is used, the system is unable to perform an injection if there are injection events in the autosampler Time program table. (ACQ-2242)	To avoid this issue, do not add injection events to the autosampler Time program table.
Inconsistent behaviour occurs during imports from an acquisition method and from a processing method, resulting in unreliable qualification results. (BLT-284)	Information imported from an acquisition method has a mass accuracy to two decimal places. Formulas used to calculate mass accuracy in a processing method produce results to four decimal places. Therefore, this might cause inconsistent results between the two methods.
The Ion source gas 2 setting is included in a user message. (MSCS-943)	When the APCI probe is used, a user message is shown stating that the Ion source gas 2 setting should be a specific value. Ignore the Ion source gas 2 settings in the user message.
Occasionally, the mass spectrometer goes to Fault state and the system cannot be recovered. (ACQ-2250)	If this issue occurs, then deactivate and reactivate the devices, and then click Standby .

Table 2-4 Acquisition (continued)

Issue	Description
The user is unable to activate the LC after it goes to Fault state. (ACQ-2207)	If this issue occurs, then clear the error on the LC, and then deactivate and activate the devices.
The Harvard syringe pump goes to Fault state when Standby is selected. (ACQ-2193)	To avoid this issue and clear the error, use the Direct Control feature to start the syringe.
An error is shown and the batch cannot be submitted if the Data File name is centered in the cell and the user presses Shift + Tab to move to the next cell. (ACQ-2135)	To avoid this issue, do not use the Tab key to move between cells. Remove the entire contents of the cell and then re-enter the required Data File name.
An incorrect message is shown when the probes are switched. (MSCS-972)	The error does not affect acquisition. Users can cancel the message and acquisition will continue.
Real time sample information is only updated when the MS Method workspace is refreshed. (MSCS-968)	To avoid this issue, close the data file and then open it post-acquisition to view the Sample Information.
The CDS remains in Wash mode after the software stops responding. (MSCS-666)	If this issue occurs, then clear the Wash mode option in the Direct Control dialog.
In the Batch workspace, the list of available MS and LC methods is incomplete if the methods are copied from a different project. (ACQ-2127)	If this issue occurs, then restart the software.
Changing polarity in the Ion Reference Table does not cause the fields to be validated. (ACQ-2186)	If the user creates a positive Ion Reference Table and then changes the polarity, the OK button is not enabled and an error is shown. If this issue occurs, then click the Negative polarity radio button, click the Positive polarity radio button, and then click the Negative polarity radio button again.
Real time updates for the DAD panel might be slower than the response time chosen in the method (DS-853)	To avoid this issue, either reduce the frequency of the DAD acquisition or inspect the data after the acquisition has completed.
A message is shown indicating that a data file is corrupted and the batch cannot be submitted. (ONYX-1539)	Occasionally, it has been observed that a batch could not be submitted because of a corrupted file message in the Batch Editor. However, when the data file is opened in the Explorer workspace, no corruption of the data file is observed. If this issue occurs, then use a different data file name for the batch or move the affected data file using Windows Explorer.

Notes on Use and Known Issues

Table 2-4 Acquisition (continued)

Issue	Description
Samples in the queue might be marked as failed even though the data is acquired successfully. (DS-1016)	During the processing of complex data during acquisition, a sample in the queue might be marked as failed even though it was acquired successfully and the queue has moved to the next sample. If this occurs, the sample and data file are not actually affected, and can be used for exploring or processing. To refresh the queue icons, restart SCIEX OS.
Acquisition is aborted when acquiring using <i>Scheduled</i> MRM ^{HR} and SWATH [®] methods or <i>Scheduled</i> MRM ^{HR} and IDA methods and the TOF MS method of the MRM HR method is deleted. (MSCS-1059)	To avoid this issue, do not delete the TOF MS experiment from the MRM HR method.
Not all of the columns shown in the UI are printed. (ACQ-2611)	Not all of the columns shown in the UI are shown in printouts of the method when the user does the following: <ol style="list-style-type: none">1. Creates an MRM method.2. Applies a scan schedule.3. Selects to show the advanced parameters.4. Saves and then prints the method. To avoid this issue, change the paper size to a size larger than Letter size.
The Calibration ID column is not shown in the Batch grid but it is shown in the exported file. (ACQ-2560)	If auto-calibration is selected, then the Column ID contains "CalibrationEnabled". If auto-calibration is not selected, then the column is shown but it does not contain any data. Data acquisition is not affected.
When data is ramped, the real time data stops updating before the end of acquisition. (ONYX-1682)	Real time and post-acquisition data do not match when parameters are ramped during acquisition. To avoid issues, use the post-acquisition data for any analysis.
Pasting data in the TOF MSMS table of an MRM HR method when the Apply Scan Schedule feature is selected hides the RT and RT Tolerance columns. (ACQ-2521)	If this issue occurs, then adjust the width of the other columns to make the two columns viewable.
During manual tuning, the optimized parameter value is not saved to instrument definition file after the user clicks Save Settings . (ACQ-2519)	During manual tuning the optimized parameter value is not saved. To avoid any issues, complete all of the tuning steps when in manual tuning mode.

Table 2-4 Acquisition (continued)

Issue	Description
The CDS pump continues to run after the calibrant sample in the queue is aborted. (MSCS-1145)	If this issue occurs, then stop the CDS manually.
When the software ramps the CE parameter during MRM generation in negative polarity, the real time Data Acquisition panel does not show spectral data and the x-axis scale is shown in positive mode. (ACQ-2727)	To avoid issues, use the MRM generator to view the results of the parameter ramp. Do not use the Real Time panel.
The Data Acquisition panel shows the previously acquired sample. (DS-1384)	If this issue occurs, then restart the software.
Pasted data is duplicated in the Batch grid. (ACQ-2713)	If data is copied and pasted from the Batch grid index using the right-click menu, then a duplicate is added to the end of the sample. To avoid any issues, either type the data or paste data from an Microsoft Excel file.
The software disregards the user choice to not proceed with a batch import. (ACQ-2704/ACQ-2705)	<p>The software disregards the user choice to not proceed with a batch import when a user does the following:</p> <ol style="list-style-type: none"> 1. Create a batch. 2. Select a non-MRM MS method and then type a sample name and data file name. Do not save the batch. 3. Click Open > Import from File. The Import a batch file dialog opens. 4. Browse to the applicable file, do not select to append the file, and then click Import. <p>The first Import warning message is shown. If the user selects No, then a second warning message is shown.</p> <p>During batch import, if the user selects No for the second warning message, then the progress bar does not close. Users must click Cancel or import the file again to close the progress bar.</p>

Notes on Use and Known Issues

Table 2-4 Acquisition (continued)

Issue	Description
<p>In the Batch and Queue workspaces, printouts using the PDFactory option have the following issues:</p> <ul style="list-style-type: none">• The date and time when other regional settings are used are not shown. (ACQ-2700)• The row index is blank when only several isolated rows are printed using PDFactory. (ACQ-2701)• If the Auto-Calibrate option is selected during batch creation, then the Calibration Sample Frequency, CDS Channel, and the Vial Position (if LC is selected for calibrant delivery) values are missing. (ACQ-2804)• Printing reports using XPS and PDFactory in Landscape mode work as expected, but when PDFactory in Portrait mode is used, the last two columns on the first page are omitted and the time at which the batch is printed is truncated and not shown in full. (ACQ-1275)	<p>To avoid any issues, print using the XPS option instead of PDFactory.</p>
<p>In the Batch and Queue workspaces, row heights on the first and second page are not consistent when either the PDFactory or the XPS option are used to print. (ACQ-2687)</p>	<p>This issue does not affect the content of the reports.</p>
<p>Peak labelling is inconsistent between XWC and TWC graphs during real time UV data acquisition. (DS-1262)</p>	<p>To avoid any issues, examine data post-acquisition using the Explorer workspace.</p>

Table 2-4 Acquisition (continued)

Issue	Description
<p>In manual tune, when the user submits a batch without any calibration sample (no CDS- or LC-autocal), the ions from the manual MS method acquisition are used as the inter-sample DBC reference list for the first sample and all the subsequent samples in the batch. If there are any mismatches in the mass range, polarity, and so forth, between the MS method used for manual acquisition and that submitted in the batch, then inter-sample calibration will fail due to mass accuracy drift for all the samples in the batch. (ACQ-2834)</p>	<p>To avoid any issues users can do one of the following:</p> <ul style="list-style-type: none"> • If the user submits a batch without any calibration sample after finishing manual acquisition in the MS Method workspace, inter-sample calibration behaves as expected. The first sample in the batch is used to generate the reference list to calibrate subsequent samples. • If the user submits a batch with a calibration sample while manual acquisition is in progress, then inter-sample calibration behaves as expected with no mass accuracy drift observed.
<p>After the user changes two numbers in the Ion Reference table and then types values in the Precursor and Fragment columns, an extra zero is added in the Ion Reference tables. For example, if the user types 12, then 120 is shown in the column.</p> <p>If the user highlights the decimal portion of Precursor or Fragment, and then start typing, the second number is entered as a zero. For example, if the original entry is 1.1111 and the user highlights 1111 and starts typing 2222, then 20222 is shown in the column. (ACQ-2832)</p>	<p>To avoid any issues, always highlight the whole number and then type the number. Do not highlight portions of the number.</p>

Notes on Use and Known Issues

Table 2-5 Analytics

Issue	Description
The expected retention time of an individual component that is part of a group (the Update Retention Time feature is set to Group) can be changed, resulting in inconsistent expected retention times and retention time windows in the group. (MQ-1511)	The user can manually change the Expected RT for each component in the group.
Changing the regression setting for one algorithm in the Project default page updates the regression setting for the other algorithm. (MQ-1376)	The regression settings fields are not independent of the algorithm selected. If the user changes a regression setting field in one algorithm, then the corresponding field in the other algorithms is also changed. To avoid any issues, when switching between algorithms, users must update the regression settings as required for the algorithm.
CSV does not support reports that contain graphics or logos. (MQ-1361)	The .csv report is supported if the report does not contain any graphics.
An error occurs when a library without a name is imported. (MQ-1379)	To avoid this issue, assign names to libraries before importing them.
The combined score is non-zero when both the Library and Search Formula Finder scores are zero or not available. (MQ-1545)	In addition to the Library Search and Formula Finder scores, the software uses the mass error, isotope, and retention time scores to calculate the combined score. To avoid including these scores, set the weighting of each to zero.
The library search reports a higher-than-expected purity score from low quality spectra. (MQ-1679) (MQ-1773)	If this issue occurs, confirm retention time, peak quality, and integration to determine if the compound is a true positive.

Table 2-5 Analytics (continued)

Issue	Description
A corrupted first sample in a data file prevents sample processing. (MQ-2118)	<p>If the first sample in a data file is corrupted, then the user is unable to process any samples in this data file and receives an informational message. A sample can become corrupted if it is aborted or fails acquisition prior to the system going to Run state during sample acquisition. If acquisition must be aborted before the system goes to Run state for the first sample, and if the data will be quantitated, then acquire the batch to a different data file. To create a Results Table using a data file that contains a corrupted sample, do the following:</p> <ol style="list-style-type: none"> 1. Create a Results Table using an uncorrupted sample from an uncorrupted batch. 2. Click Process > Add Samples. 3. Select all of the samples for the corrupted batch except the first corrupted sample. 4. Click OK. The corrupted batch is added to the Results Table. 5. Remove the uncorrupted sample from the original batch by clicking Process > Remove Selected Samples. 6. Process the batch as normal.
Licences for licensed packages created with LibraryView Package Builder are saved to C:\Program Files\AB SCIEX\LibraryView\bin. (MQ-1847)	Licences for the licensed packages created with LibraryView Package Builder 1.0 should be manually copied to C:\Program Files\SCIEX\LibraryView\LibraryViewFramework\Server.
Compound-specific acceptance criteria are not available. (MQ-1822)	Currently, only the global settings are available for Library Search.
The default CES library search selection results in missed hits in non-CES data. MQ-1805)	If this issue occurs, then clear the Collision Energy Spread check box from the search algorithm.

Table 2-5 Analytics (continued)

Issue	Description
Real time updates might be delayed when creating Results Tables. (DS-1042)	Delays are observed when the user runs acquisitions or processes data containing a large number of experiments. To avoid any issues, do one of the following: <ul style="list-style-type: none"> • Reduce the number of experiments that are being acquired. • Reduce the number of experiments used to generate the Results Table. • Avoid generating Results Tables and acquiring data concurrently.
Incompatible components in the embedded AutoPeak method are not handled correctly. (MQ-1873)	When an existing AutoPeak method is used to process data with the option to create a model using the currently selected sample, the Results Table opens correctly. However, incompatible components are shown with a red exclamation mark in the embedded method. Users can remove the incompatible components from the method or they can modify the fragment mass retention time or experiment index to avoid this behavior.
The software stops responding when the Summation algorithm method contains incompatible components. (MQ-1888)	If an existing Summation algorithm method is used and if the method is not completely compatible with the data, then the software will stop responding. If this issue occurs, then edit the method to remove the incompatible components.
Saved Results Tables are not automatically updated when a library is added or removed from the database. (MQ-1684)	To avoid any issues, manually reprocess the results based on the updated library database.
Some chromatograms are not shown when the Peak Review pane is opened. (MQ-2070)	If this issue occurs, then click an index in the Results Table.
Potential extra time is added to random cycles during IDA acquisition. (ONYX-1764)	To avoid any issues, make sure that the Google update services (gupdate and gupdatem), if present on the system, as well as Windows backup, are disabled before running IDA.
After the Analytics workspace is closed by clicking the blue X in the top right corner, the Samples pane and the Components and Groups pane are not refreshed when the workspace and Result Table are opened again. (MQ-2074)	If this issue occurs, then click anywhere on the screen to refresh the panes.

Table 2-5 Analytics (continued)

Issue	Description
During any looped or combined experiments, a dual subtracted MS/MS spectrum is shown in the Peak Review pane. (MQ-1848)	This is not an issue and the software is working as designed. A single IDA experiment will have only a single subtracted spectrum range.
AutoPeak results generated on different computers that have different CPU architectures show a difference at the eleventh digit. (MQ-2316)	Users can customize the Results Table view. In an open Results Table, click More > Results Tables > Display settings and set the Number Format field to a value that is less than 11. Users will notice differences in their results if the value is 11 or higher.
The IS Name cannot be pasted in the Components Table in the Method Editor. (MQ-2193)	To avoid issues, either manually select the IS Name or paste the IS column separately.
The user is prompted to save changes to the Results Table even if no changes were made. (MQ-2400)	If the user moves a qsession file to another folder, and then opens and closes the Results Table without making any changes, the software prompts the user to save the changes. Users can select either Save or Cancel . Data analysis is not affected.
The software seems unresponsive when PDFactory is used to create a protected PDF report from a Results Table that contains more than 2500 rows using the Positive Hit template docx. (MQ-1896)	Creating the report can take some time. The PDFactory progress window, which is always shown in the background, shows that the PDF creation is in progress. Users can minimize all of the windows, including SCIEX OS, to view the PDFactory progress window.
Users are able to process and create Results Table with an invalid method. (MQ-2431)	To avoid any issues, users must open methods created in earlier versions of SCIEX OS and correct any errors. If errors are not corrected, then processing time might be impacted.
If the user processes data while the system acquires data, then large temp files might be created that impact system performance. (ACQ-2382)	If the system stops responding while acquiring and processing data on the same computer, then delete the \\Update\Local\Temp file located on the C drive.

Table 2-6 Explorer

Issue	Description
<p>The following issues can occur when the user explores data during acquisition:</p> <ul style="list-style-type: none"> • Real time data does not match the post-acquisition data if the XICs and BPCs for scheduled scans are generated before the scheduled time. (DS-903/ DS-1092) • If the user toggles between MS experiments using the Move to next or Move to previous button in Explorer to show XIC/BPC generated in real time, only one point is shown in the XIC/BPC pane. 	<p>To avoid this issue, do the following:</p> <ul style="list-style-type: none"> • Generate XICs for the required experiment using the File > Show XIC • Generate the XIC/BPC post-acquisition. • Close the XIC pane and reopen it.
<p>The number label in an XIC trace is misleading in the Explorer workspace. (PV-1009)</p>	<p>The value shown is correct because it represents the centroid value of the peak (use the Fill Peaks button for a better view of the peak). The peak label is placed on the highest point of the peak in question regardless of its position. Therefore, the label might seem to be in the incorrect position, but the value is correct.</p>
<p>The number label in an XIC trace is misleading in the Explorer workspace. (PV-1009)</p>	<p>If this issue starts to occur, then wait for the acquisition to complete before exploring the data.</p>
<p>Updates to the real time data spectra shown in the MS and DAD tabs in the data acquisition panel might be slower than in the Explorer workspace. (DS-934)</p> <p>A mismatch in the real time graph in the MS and DAD acquisition panels and in the Explorer workspace occurs when the LC method duration is longer than the MS method. In this scenario, both the MS and DAD acquisition panels stop updating at the end of MS method duration, even though the UV, DAD, or ADC channel continues to update in real time in the Explorer workspace until the end of the LC method acquisition time. (DS-852)</p>	<p>The x-axis (Detector Voltage) is labelled incorrectly. To avoid any issue, use the Detector Optimization Report or the Data Acquisition panel to inspect the data acquired during the detector optimization process.</p>
<p>Detector optimization data is not shown correctly in the Explorer workspace. (DS-1044)</p>	<p>Although the software generates an error, all of the samples are opened. The user can remove the corrupted sample from the batch.</p>

Table 2-6 Explorer (continued)

Issue	Description
Incorrect precursor charge might be shown in the IDA Explorer and survey scan spectrum. (MSCS-1117)	This issue does not affect decision making during IDA acquisition.
Real time sample data can be used to recalibrate the sample. (DS-1094)	To avoid any issues, recalibrate the sample post-acquisition.
The user is unable to generate a spectrum from a highlighted region in the XIC. (ONYX-1882)	<p>An error message is shown when a user does the following:</p> <ol style="list-style-type: none"> 1. Open two files in separate panes in the Explorer workspace and then generate an XIC graph for each file. 2. Combine the XIC graphs in a single pane. 3. In the XIC pane, highlight a region and then double-click to generate a spectrum. 4. In the Process All Overlays? dialog that opens, click All Overlaid and then click OK. The error message "Incorrect Argument - invalid cycle range" is shown instead of the spectrum. <p>To avoid any issues, select a narrower region where the graphs are overlapped.</p>
Data files opened in the Explorer workspace in real time do not show the correct sample number from the batch. (DS-1340)	If this issue occurs, then open the file after the acquisition is complete.
When a user processes large amounts of data or multiple data files in the Explorer workspace, the user interface might stop responding and there could be delay before the sample queue moves to the next sample. (ONYX-2047/DS-1688)	If this issue occurs, then wait for the software to finish processing in the Explorer workspace or avoid processing a large amount of data during data acquisition.
SCIEX OS stops responding or generates an error when the user tries to simultaneously generate a DAD contour plot and XWC in a IDA+DAD datafile. This issue only occurs when the user has started to generate a DAD contour panel and while it is updating in the background, the user accesses a XWC at the same time. (BLT-498)	<p>If this issue occurs, then do one of the following:</p> <ul style="list-style-type: none"> • Generate the XWC first and then generate the DAD contour panel. • Wait until the contour panel has finished updating before generating the XWC.

Notes on Use and Known Issues

Table 2-7 MS Tune

Issue	Description
When the Q1 center mass is selected, the mass range of the real time spectrum is not updated accordingly. (DS-915)	To avoid this issue, set the start and stop masses to cover the Q1 center mass range.
An MS Tune acquisition event continues after the user navigates away from workspace. (ACQ-2113)	If this issue occurs, then stop the acquisition from the Queue workspace.
When the Advanced Troubleshooting feature is opened for the first time, the user interface shows the Nebulizer Current parameter instead of the Spray Voltage parameter. (ONYX-2086)	After acquisition starts, the user interface is refreshed and the correct parameters are shown. At this point, set the required Spray Voltage parameter.

Table 2-8 Software Installation

Issue	Description
The SCIEX OS might fail to install if an incorrect user account is used. (BLT-340)	If this issue occurs, then contact sciex.com/request-support . Only Administrators should install or remove the software.
The SCIEX OS fails to install if more than one instance of the Installation Wizard is open. (BLT-341)	If two instances of the SCIEX OS Installation Wizard are opened, and the user attempts to proceed with the installation from the second instance (regardless of whether or not the first instance is closed), then the installation fails. To avoid this issue, open only a single instance of the Installation Wizard and then proceed with the installation.

Revision History

Revision	Reason for Change	Date
A	First release of document.	February 2016
B	Added the following sections: <ul style="list-style-type: none">• New Features and Fixes from Version 1.0 to Version 1.1• Install the BioPharmaView Software Updated the following sections: <ul style="list-style-type: none">• Notes on Use and Known Issues• Install the Software• Mass Spectrometer Firmware Versions• Mass Spectrometer Configuration Table	October 2016
C	Revised to add features and issues for version 1.2.	February 2017